

2,2,2-Trifluoroethanol
75-89-8 | DTXSID0021751

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 79.7 °C

Global applicability domain: Inside

Local applicability domain index: 5.12e-01

Confidence level: 7.42e-01

Nearest Neighbors from the Training Set

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2,2,2-Trifluoroethanol

Measured: 74.0

Predicted: 79.7

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1-Propanol, 2,2,3,3-tetrafluoro-

Measured: 110

Predicted: 102

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1,1,1-Trifluoro-2-propanol

Measured: 75.5

Predicted: 86.4

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Difluoroethanol

Measured: 95.5

Predicted: 93.6